

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of atrazine is located in Table 4-1.

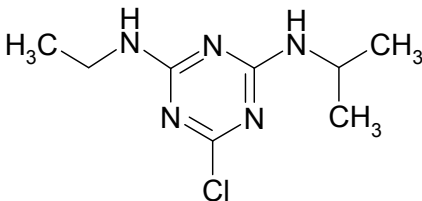
Atrazine is produced commercially in the United States as a technical-grade chemical with a purity of 92–97% (IARC 1999) to 99.9% (EPA 1983) active ingredient. Impurities in the former formulation included dichlorotriazines, hydroxytriazines and tris(alkyl)aminotriazines.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of atrazine is located in Table 4-2.

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Table 4-1. Chemical Identity of Atrazine

Characteristic	Information	Reference
Chemical name:	Atrazine	EPA 1983; Howard 1991
Synonyms:	6-Chloro-n-ethyl-n'-(1-methylethyl)-triazine-2,4-diamine; 2-Chloro-4-ethyl-amino-6-iso-propylamine-s-triazine; 2-Chloro-4-(ethyl-amino)-6-(isopropyl-amino)-s-triazine; 2-Chloro-4-(ethyl-amino)-6-(isopropylamino)triazine; Chloro-4-(propylamino)-6-ethyl-amino-s-triazine; Chloro-3-ethylamino-5-isopropyl-amino-2,4,6-triazine; Butyl-n-(acetyl)-aminopropionic acid	
Registered trade names:	Aatrex®, Aatram®, Atratol®, Gesaprim®	EPA 1983 (PB84-149541); Syngenta 2000
Chemical structure:		
Identification numbers:		
CAS registry	1912-24-9	HSDB 2001
NIOSH RTECS	XY5600000	HSDB 2001
DOT/UN/NA/IMO	UN 2763	HSDB 2001
	UN 2997	HSDB 2001
	UN 2764	HSDB 2001
	UN 2998	HSDB 2001
	IMO 6.1	HSDB 2001
	IMO 3.2	HSDB 2001
HSDB	413	HSDB 2001
Experimental code number	G-30027 (Ciba-Geigy)	Farm Chem Handbook 2001

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of Atrazine

Property	Information	Reference
Molecular weight	215.69	HSDB 2001
Color	White colorless	HSDB 2001
Physical state	Colorless powder Colorless crystals	IARC 1999 Verschuereen 2001
Melting point	173–175 °C	HSDB 2001
Density	1.23 g/cm ³ (22 °C)	HSDB 2001
Odor	Odorless	NIOSH 1994
Solubility:		
at 22 EC	Soluble in water (34.7 mg/L)	Ward and Weber 1968
at 25 EC	Soluble in ethylacetate (24 g/L), acetone (31 g/L), dichloromethane (28 g/L), ethanol (15 g/L), toluene (4 g/L), n-hexane (0.11 g/L), and n-octanol (8.7 g/L)	Tomlin 1997
at 27 EC	Soluble in n-pentane (360 mg/L), diethyl ether (12,000 mg/L), methanol (18,000 mg/L), ethyl acetate (28,000 mg/L), chloroform (52,000 mg/L), and dimethyl sulfoxide (183,000 mg/L)	Humburg 1999
Partition coefficients:		
Log K _{ow}	2.60 2.71	Hansch et al. 1995 Brown and Flagg 1981
Log K _{oc}	1.96 1.97 2.98 3.38 2.18 2.53 2.33	Dousset et al. 1994 Green et al. 1993 Koskinen and Rochette 1996 Koskinen and Rochette 1996 Meakins et al. 1995 Meakins et al. 1995 Weber 1991
Vapor pressure at 25 EC	2.89x10 ⁻⁷ mmHg	Tomlin 1997
Henry's law constant at 25 EC	2.96x10 ⁻⁹ atm-m ³ /mol	Reiderer 1990
pK _a	1.68	Bailey et al. 1968
Hydrolysis rate constant at 25 EC	2.735x10 ⁻¹¹ cm ³ /molecule-second (estimated)	Meylan and Howard 1993
Autoignition temperature	No data	

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Table 4-2. Physical and Chemical Properties of Atrazine (*continued*)

Property	Information	Reference
Flashpoint	Not applicable	EPA 1983
Flammability limits	Not applicable	EPA 1983
Conversion factors ^a	mg/m ³ =8.82xppm	HSDB 2001; IARC 1999
Explosive limits	not applicable	EPA 1983

^aIn air, atrazine is both present in the gas phase and associated with particulates (HSDB 2001). Conversion factors are only applicable for those compounds that exist entirely in the vapor phase. Therefore, while this conversion factor has been reported in the literature, its use is not recommended, as it will not provide an accurate reflection of ambient air atrazine concentrations.